

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptajsl1623

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\*\*\*\*\* Welcome to STN International \*\*\*\*\*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 JAN 02 STN pricing information for 2008 now available  
NEWS 3 JAN 16 CAS patent coverage enhanced to include exemplified  
prophetic substances  
NEWS 4 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new  
custom IPC display formats  
NEWS 5 JAN 28 MARPAT searching enhanced  
NEWS 6 JAN 28 USGENE now provides USPTO sequence data within 3 days  
of publication  
NEWS 7 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment  
NEWS 8 JAN 28 MEDLINE and LMEEDLINE reloaded with enhancements  
NEWS 9 FEB 08 STN Express, Version 8.3, now available  
NEWS 10 FEB 20 PCI now available as a replacement to DPCI  
NEWS 11 FEB 25 IFIREF reloaded with enhancements  
NEWS 12 FEB 25 IMSPRODUCT reloaded with enhancements  
NEWS 13 FEB 29 WFINDEX/WFIDS/WPIX enhanced with ECLA and current  
U.S. National Patent Classification  
NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom  
IPC display formats  
NEWS 15 MAR 31 CAS REGISTRY enhanced with additional experimental  
spectra  
NEWS 16 MAR 31 CA/CAPLUS and CASREACT patent number format for U.S.  
applications updated  
NEWS 17 MAR 31 LPCI now available as a replacement to LDPCI  
NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements  
NEWS 19 APR 04 STN AnaVist, Version 1, to be discontinued  
NEWS 20 APR 15 WPIDS, WFINDEX, and WPIX enhanced with new  
predefined hit display formats  
NEWS 21 APR 28 EMBASE Controlled Term thesaurus enhanced  
NEWS 22 APR 28 IMSRESEARCH reloaded with enhancements  
  
NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that  
specific topic.

All use of STN is subject to the provisions of the STN Customer  
agreement. Please note that this agreement limits use to scientific

research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 10:24:37 ON 28 MAY 2008

=> b res		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'DISSABS' ENTERED AT 10:24:51 ON 28 MAY 2008

COPYRIGHT (C) 2008 ProQuest Information and Learning Company; All Rights Reserved.

FILE 'DKF' ENTERED AT 10:24:51 ON 28 MAY 2008

COPYRIGHT (C) 2008 Dokumentation Kraftfahrwesen e.V., Germany

FILE 'NTIS' ENTERED AT 10:24:51 ON 28 MAY 2008

Compiled and distributed by the NTIS, U.S. Department of Commerce.

It contains copyrighted material.

All rights reserved. (2008)

FILE 'SOFIS' ENTERED AT 10:24:51 ON 28 MAY 2008

COPYRIGHT (C) 2008 GESIS-IZ Sozialwissenschaften, Bonn

FILE 'SOLIS' ENTERED AT 10:24:51 ON 28 MAY 2008

COPYRIGHT (C) 2008 GESIS-IZ Sozialwissenschaften, Bonn

FILE 'UFORDAT' ENTERED AT 10:24:51 ON 28 MAY 2008

COPYRIGHT (C) 2008 Umweltbundesamt, D-14191 Berlin (UBA)

=> b reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.45	7.66

FILE 'REGISTRY' ENTERED AT 10:24:54 ON 28 MAY 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 MAY 2008 HIGHEST RN 1023132-78-6

DICTIONARY FILE UPDATES: 27 MAY 2008 HIGHEST RN 1023132-78-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> e 488-59-5/rn

E1	1	488-55-1/RN
E2	1	488-58-4/RN
E3	1 -->	488-59-5/RN
E4	1	488-64-2/RN
E5	1	488-65-3/RN
E6	1	488-66-4/RN
E7	1	488-67-5/RN
E8	1	488-68-6/RN
E9	1	488-69-7/RN
E10	1	488-70-0/RN
E11	1	488-71-1/RN
E12	1	488-73-3/RN

=> s e3

L1 1 488-59-5/RN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 488-59-5 REGISTRY

ED Entered STN: 16 Nov 1984

CN scyllo-Inositol (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Inositol, scyllo- (8CI)

CN Scyllitol (6CI, 7CI)

OTHER NAMES:

CN AZD 103

CN Cocositol

CN Quercinitol

CN scyllo-Cyclohexanehexol

FS STEREOSEARCH

DR 887751-76-0

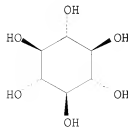
MF C6 H12 O6

CI COM

LC STN Files: ADISINSIGHT, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DDFU, DRUGU, EMBASE, GMELIN\*, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, NAPRALERT, PROUSDDR, SPECINFO, TOXCENTER, USPAT2, USPATFULL, USPATOLD

(\*File contains numerically searchable property data)

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

363 REFERENCES IN FILE CA (1907 TO DATE)  
8 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
364 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
23 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> b caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.46	10.12

FILE 'CAPLUS' ENTERED AT 10:25:24 ON 28 MAY 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 28 May 2008 VOL 148 ISS 22  
FILE LAST UPDATED: 27 May 2008 (20080527/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

```
=> s l1 and prep/rl
      364 L1
      4578676 PREP/RL
L2      86 L1 AND PREP/RL

=> s l2 and (bor?)
      661159 BOR?
L3      16 L2 AND (BOR?)

=> s l3 and py<=2004
      25083718 PY<=2004
L4      15 L3 AND PY<=2004

=> s l3 and inosose
      350 INOSOSE
      32 INOSOSES
      356 INOSOSE
          (INOSOSE OR INOSOSES)
L5      9 L3 AND INOSOSE
```

=> d 15 1-9 ibib abs hit

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:347182 CAPLUS

DOCUMENT NUMBER: 142:372560

TITLE: Enzymic manufacture of scyllo-inositol from  
myo-inositol and manufacture of scyllo-inositol from  
myo-inositol

INVENTOR(S): Yamaguchi, Masanori; Kita, Yuichi; Mori, Tetsuya;  
Kanbe, Kenji; Tomoda, Akihiro; Takahashi, Atsushi;  
Ichikawa, Wakako

PATENT ASSIGNEE(S): Hokko Chemical Industry Co., Ltd., Japan

SOURCE: PCT Int. Appl., 117 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005035774	A1	20050421	WO 2004-JP15174	20041014
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2542560	A1	20050421	CA 2004-2542560	20041014
EP 1674578	A1	20060628	EP 2004-817164	20041014
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
CN 1867676	A	20061122	CN 2004-80030178	20041014
US 20060240534	A1	20061026	US 2006-576030	20060413
IN 2006CN01666	A	20070629	IN 2006-CN1666	20060512
PRIORITY APPLN. INFO.:			JP 2003-353490	A 20031014
			JP 2003-353491	A 20031014
			JP 2004-18128	A 20040127
			JP 2004-194088	A 20040630
			WO 2004-JP15174	W 20041014

AB Scyllo-inositol is manufactured from myo-inositol by enzymes containing NAD<sup>+</sup>-independent myo-inositol dehydrogenase and scyllo-inositol dehydrogenase. The myo-inositol is first converted to scyllo-inosose and then to scyllo-inositol. Alternatively, scyllo-inositol is manufactured from myo-inositol with Burkholderia or Acetobacter. The scyllo-inositol may be isolated from the reaction mixture or fermentation broth by boric acid and metal salts.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB Scyllo-inositol is manufactured from myo-inositol by enzymes containing NAD<sup>+</sup>-independent myo-inositol dehydrogenase and scyllo-inositol dehydrogenase. The myo-inositol is first converted to scyllo-inosose and then to scyllo-inositol. Alternatively, scyllo-inositol is manufactured from myo-inositol with Burkholderia or

Acetobacter. The scyllo-inositol may be isolated from the reaction mixture or fermentation broth by boric acid and metal salts.

IT 488-59-5P, scyllo-Inositol

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(enzymic manufacture of scyllo-inositol from myo-inositol and manufacture of scyllo-inositol from myo-inositol)

IT 488-64-2P, scyllo-Inosose

RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(enzymic manufacture of scyllo-inositol from myo-inositol and manufacture of scyllo-inositol from myo-inositol)

IT 144-55-8, Sodium bicarbonate, biological studies 298-14-6, Potassium bicarbonate 497-19-8, Sodium carbonate, biological studies 546-93-0, Magnesium carbonate 1303-96-4, Borax 7447-40-7, Potassium chloride, biological studies 7487-88-9, Magnesium sulfate, biological studies 7558-79-4, Sodium monohydrogen phosphate 7558-80-7, Sodium dihydrogen phosphate 7601-54-9, Trisodium phosphate 7646-93-7, Potassium bisulfate 7647-01-0, Hydrochloric acid, biological studies 7647-14-5, Sodium chloride, biological studies 7681-38-1, Sodium hydrogen sulfate 7757-82-6, Sodium sulfate, biological studies 7758-11-4, Potassium monohydrogen phosphate 7778-53-2, Tripotassium phosphate 7778-77-0, Potassium dihydrogen phosphate 7778-80-5, Potassium sulfate, biological studies 7786-30-3, Magnesium chloride, biological studies 10043-35-3, Boric acid, biological studies  
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(enzymic manufacture of scyllo-inositol from myo-inositol and manufacture of scyllo-inositol from myo-inositol)

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:287066 CAPLUS

DOCUMENT NUMBER: 140:304023

TITLE: Preparation of scyllo-inositol with high stereoselectivity

INVENTOR(S): Takahashi, Yoshiaki; Miyake, Toshiaki; Saotome, Hiromi; Yamaguchi, Masanori; Takahashi, Atsushi

PATENT ASSIGNEE(S): Hokko Chemical Industry Co., Ltd., Japan; Microbiochemical Research Foundation

SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004107287	A	20040408	JP 2002-274716	20020920
PRIORITY APPLN. INFO.:			JP 2002-274716	20020920
OTHER SOURCE(S):	MARPAT 140:304023			

AB The compound, useful as a material for Anti-Alzheimer's agents and liquid crystal compds. (no data), is prepared by protection of 5 OH groups in scyllo-inosose with organosilyl compds. or halo-, alkoxy-, or aryloxy-(un)substituted lower alkanoyl compds., reduction of OH-protected scyllo-inosose with boron hydride-type reducing agents or Ni catalysts and H<sub>2</sub>, recovery of OH-protected scyllo-inositol and myo-inositol from the reaction mixts., deprotection, recovery of

scyllo-inositol and myo-inositol, and separation of them. 1,3,4,5,6-Penta-O-triorganosilyl-scyllo-inositols are prepared as intermediates. Purification processes of scyllo-inosose from their aqueous solution are also described. An aqueous solution containing 10% scyllo-inosose was subjected to evaporation to dryness at 76°, reacted with Me3SiCl in pyridine and AcOEt at 50° for 30 min, reduced with NaBH4 in MeOH-hexane at room temperature for 30 min, deprotected with HCl for 30 min, and recrystd. in H2O-EtOH to give 79% scyllo-inositol without myo-inositol.

AB The compound, useful as a material for Anti-Alzheimer's agents and liquid crystal compds. (no data), is prepared by protection of 5 OH groups in scyllo-inosose with organosilyl compds. or halo-, alkoxy-, or aryloxy-(un)substituted lower alkanoyl compds., reduction of OH-protected scyllo-inosose with boron hydride-type reducing agents or Ni catalysts and H, recovery of OH-protected scyllo-inositol and myo-inositol from the reaction mixts., deprotection, recovery of scyllo-inositol and myo-inositol, and separation of them. 1,3,4,5,6-Penta-O-triorganosilyl-scyllo-inositols are prepared as intermediates. Purification processes of scyllo-inosose from their aqueous solution are also described. An aqueous solution containing 10% scyllo-inosose was subjected to evaporation to dryness at 76°, reacted with Me3SiCl in pyridine and AcOEt at 50° for 30 min, reduced with NaBH4 in MeOH-hexane at room temperature for 30 min, deprotected with HCl for 30 min, and recrystd. in H2O-EtOH to give 79% scyllo-inositol without myo-inositol.

ST scyllo inosose protection organosilyl compd; alkanoyl compd protection scyllo inosose; silyl protected inosose stereoselective redn boron hydride; nickel catalyst stereoselective hydrogenation alkanoyl inosose; inositol scyllo stereoselective prepn; sodium borohydride stereoselective redn scyllo methylsilylinosose; acetylinosose scyllo stereoselective hydrogenation catalyst nickel

IT Silanes  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(halosilanes, organic, protecting compound; preparation of scyllo-inositol

by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)

IT Polar solvents  
(mixts. with nonpolar solvents, solvents in reduction; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)

IT Solvents  
(nonpolar, mixts. with polar solvents, solvents in reduction; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)

IT Asymmetric synthesis and induction  
Asymmetric synthesis and induction catalysts  
(preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)

IT Alcohols, uses  
Esters, uses  
RL: NUU (Other use, unclassified); USES (Uses)  
(solvents in reduction; preparation of scyllo-inositol by protection of

scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)

IT Hydrogenation catalysts

## Reduction

- (stereoselective; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 110-54-3, Hexane, uses  
RL: NUU (Other use, unclassified); USES (Uses)  
(mixture with MeOH, solvent in reduction; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 488-59-5P, scyllo-Inositol  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 488-64-2P, scyllo-Inosose  
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 676655-70-2P 676655-71-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 75-77-4, Trimethylsilyl chloride, reactions 108-24-7, Acetic anhydride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(protecting compound; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 16940-66-2, Sodium tetrahydroborate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reducing agent; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 13283-31-3D, Boron hydride, salts  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reducing agents; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 7440-02-0, Nickel, uses  
RL: CAT (Catalyst use); USES (Uses)  
(reducing catalyst; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 64-17-5, Ethanol, uses 67-64-1, Acetone, uses  
RL: NUU (Other use, unclassified); USES (Uses)  
(solvent for purification of inosose; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)
- IT 67-56-1, Methanol, uses 141-78-6, Ethyl acetate, uses  
RL: NUU (Other use, unclassified); USES (Uses)  
(solvent in reduction; preparation of scyllo-inositol by protection of scyllo-inosose with organosilyl compds. or lower alkanoyl compds., stereoselective reduction, and deprotection)



L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:266870 CAPLUS

DOCUMENT NUMBER: 138:270409

TITLE: Scyllo-inosose and scyllo-inositol  
manufacture

INVENTOR(S): Kamibe, Kenji; Takahashi, Atsushi; Kita, Yuichi;  
Yamaguchi, Masanori; Tamamura, Takeshi; Mori, Tetsuya

PATENT ASSIGNEE(S): Hokko Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003102492	A	20030408	JP 2002-184912	20020625
JP 3981597	B2	20070926		

PRIORITY APPLN. INFO.: JP 2001-191161 A 20010625

AB The scyllo-inosose is manufactured from myo-inositol with Pseudomonas and Acetobacter. The scyllo-inosose is reduced with an reductant such as sodium borohydride to get scyllo-inositol. The physiol. and morphol. characteristics of these microorganisms were given. The scyllo-inosose is an useful intermediate for manufacturing pharmaceuticals. The scyllo-inositol is useful for control of. Alzheimer disease and for prepared liquid crystal.

TI Scyllo-inosose and scyllo-inositol manufacture

AB The scyllo-inosose is manufactured from myo-inositol with Pseudomonas and Acetobacter. The scyllo-inosose is reduced with an reductant such as sodium borohydride to get scyllo-inositol. The physiol. and morphol. characteristics of these microorganisms were given. The scyllo-inosose is an useful intermediate for manufacturing pharmaceuticals. The scyllo-inositol is useful for control of. Alzheimer disease and for prepared liquid crystal.

ST scyllo inosose manuf myoinositol Pseudomonas Acetobacter; redn  
scyllo inositol Alzheimer disease pharmaceutical

IT Acetobacter

Alzheimer's disease

Fermentation

Liquid crystals

Pseudomonas

Reducing agents

(scyllo-inosose and scyllo-inositol manufacture)

IT 488-64-2P, scyllo-inosose

RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL

(Biological study); PREP (Preparation); USES (Uses)

(scyllo-inosose and scyllo-inositol manufacture)

IT 87-89-8, myo-Inositol

RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(scyllo-inosose and scyllo-inositol manufacture)

IT 16940-66-2, Sodium borohydride

RL: RCT (Reactant); RACT (Reactant or reagent)

(scyllo-inosose and scyllo-inositol manufacture)

IT 488-59-5P, scyllo-Inositol

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(scyllo-inosose and scyllo-inositol manufacture)

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1986:130221 CAPLUS  
DOCUMENT NUMBER: 104:130221  
ORIGINAL REFERENCE NO.: 104:20621a,20624a  
TITLE: Scyllo-inositol  
INVENTOR(S): Praefcke, Klaus; Kohne, Bernd  
PATENT ASSIGNEE(S): Merck Patent G.m.b.H. , Fed. Rep. Ger.  
SOURCE: Ger. Offen., 10 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	DE 3405663	A1	19850822	DE 1984-3405663	19840217
	JP 60248637	A	19851209	JP 1985-26630	19850215
PRIORITY APPLN. INFO.:				DE 1984-3405663	A 19840217
AB	The title compound (I) was prepared from myo-inositol (II) in a 4 step process by oxidation of II with mol. O using a reduced PtO catalyst, acetylation of the resulting myo- <u>inosose</u> , reduction of the penta-O-acetyl-myo- <u>inosose</u> with NaBH <sub>4</sub> in MeOH, and deacetylation.				
AB	The title compound (I) was prepared from myo-inositol (II) in a 4 step process by oxidation of II with mol. O using a reduced PtO catalyst, acetylation of the resulting myo- <u>inosose</u> , reduction of the penta-O-acetyl-myo- <u>inosose</u> with NaBH <sub>4</sub> in MeOH, and deacetylation.				
ST	myo inositol oxidn; <u>inosose</u> pentaacetyl redn <u>borohydride</u>				
IT	488-64-2P RL: RCT (Reactant); SPN (Synthetic preparation); <u>PREP</u> ( <u>Preparation</u> ); RACT (Reactant or reagent) (preparation and acetylation of)				
IT	20097-56-7P RL: RCT (Reactant); SPN (Synthetic preparation); <u>PREP</u> ( <u>Preparation</u> ); RACT (Reactant or reagent) (preparation and reduction and deacetylation of)				
IT	488-59-5P RL: SPN (Synthetic preparation); <u>PREP</u> ( <u>Preparation</u> ) (preparation of, from myo-inositol, by oxidation-reduction process)				

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1985:406642 CAPLUS  
DOCUMENT NUMBER: 103:6642  
ORIGINAL REFERENCE NO.: 103:1203a,1206a  
TITLE: Note on the preparation of scyllo-inositol  
AUTHOR(S): Kohne, Bernd; Praefcke, Klaus  
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Berlin, Berlin,  
D-1000/12, Fed. Rep. Ger.  
SOURCE: Liebigs Annalen der Chemie (1985), (4), 866-8  
CODEN: LACHDL; ISSN: 0170-2041  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 103:6642  
AB A simplified synthesis of scyllo-inositol from myo-inositol via myo-inosose pentaacetate is described.  
AB A simplified synthesis of scyllo-inositol from myo-inositol via myo-

*inosose* pentaacetate is described.

IT 87-89-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidation of, to *inosose* in presence of platinum(II) oxide)

IT 488-64-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
 (preparation and acetylation of)

IT 20097-56-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
 (preparation and borohydride reduction of)

IT 488-59-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, from myo-inositol)

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:570714 CAPLUS

DOCUMENT NUMBER: 91:170714

ORIGINAL REFERENCE NO.: 91:27513a,27516a

TITLE: Intermediates in the myo-inositol 1-phosphate synthase reaction

AUTHOR(S): Eisenberg, Frank, Jr.

CORPORATE SOURCE: Natl. Inst. Arthritis, Metabl. Dig. Dis., NIH, Bethesda, MD, 20014, USA

SOURCE: Cyclitols Phosphoinositides, [Proc. Symp.] (1978), Meeting Date 1977, 269-78. Editor(s): Wells, William W.; Eisenberg, Frank, Jr. Academic: New York, N. Y. CODEN: 40YTAT

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Two lines of evidence, both indirect, are presented to support an internal aldol condensation mechanism in the oxido-reductive conversion of glucose 6-phosphate into myo-inositol 1-phosphate, catalyzed by myo-inositol 1-phosphate synthase and NAD. Comparison of enzymic reaction rates among variously 2H-labeled glucose 6-phosphates suggests activation at C5, consistent with the aldol mechanism. The addition of NaBH4 to a synthesizing system led to the isolation of epimeric inositol-3H and scyllo-inositol-3H, consistent with the formation of myo-inosose -2 1-phosphate, an intermediate postulated by the aldol mechanism. Addnl., tech. innovations in the gas chromatog. separation of iditol and glucitol, the epimers expected from NaBH4 reduction of 5-ketoglucose 6-phosphate, another postulated intermediate, are presented.

AB Two lines of evidence, both indirect, are presented to support an internal aldol condensation mechanism in the oxido-reductive conversion of glucose 6-phosphate into myo-inositol 1-phosphate, catalyzed by myo-inositol 1-phosphate synthase and NAD. Comparison of enzymic reaction rates among variously 2H-labeled glucose 6-phosphates suggests activation at C5, consistent with the aldol mechanism. The addition of NaBH4 to a synthesizing system led to the isolation of epimeric inositol-3H and scyllo-inositol-3H, consistent with the formation of myo-inosose -2 1-phosphate, an intermediate postulated by the aldol mechanism. Addnl., tech. innovations in the gas chromatog. separation of iditol and glucitol, the epimers expected from NaBH4 reduction of 5-ketoglucose 6-phosphate, another postulated intermediate, are presented.

IT 488-59-5  
 RL: FORM (Formation, nonpreparative)  
 (formation of, in inositol phosphate synthase reaction after borohydride redn)

IT 71716-43-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)  
IT 3470-36-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with deuterated sodium borohydride)  
IT 1198-69-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of, with borohydride)

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:92501 CAPLUS  
DOCUMENT NUMBER: 52:92501  
ORIGINAL REFERENCE NO.: 52:16223h-i,16224a  
TITLE: Scyllitol diborate  
AUTHOR(S): Weissbach, Arthur  
CORPORATE SOURCE: Natl. Insts. of Health, Bethesda, MD  
SOURCE: Journal of Organic Chemistry (1958), 23, 329-30  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB Theoretically the all-axial conformation of scyllitol (I) could form a double tridentate complex (II) with borate. In support of this hypothesis, II has now been isolated. The reduction of scyllo-myo-inosose with NaBH<sub>4</sub> was reported (Reymond, C.A. 51, 12024c) to yield 32% I and 45% myoinositol (III). During this reduction the present author noted a white solid that began to precipitate from the mixture, and

after 24-36 hrs. this precipitate was collected, washed with H<sub>2</sub>O and dried to give

0.9 g. crude II. II was distinguished from I, III, and the starting material by paper chromatography. II migrated twice as fast as III on paper ionophoresis in 0.125M Na borate. I in this ionophoresis shows no migration. II is nonreducing in Fehling or Park-Johnson tests. II with Ac<sub>2</sub>O and H<sub>2</sub>SO<sub>4</sub> gave 60-70% I hexaacetate, m. 286°. III hexaacetate was not detected. II acidified with H<sub>2</sub>SO<sub>4</sub>, the resultant solution repeatedly evaporated with MeOH, the residue taken up in H<sub>2</sub>O,

deionized with Amberlite MB-3, and the eluate again taken to dryness gave I. II would appear to be a monohydrate. I heated at 100° with 0.125M borate gave a compound migrating at the same rate as II. The stereochemistry of II is still unproved and is being further investigated.

AB Theoretically the all-axial conformation of scyllitol (I) could form a double tridentate complex (II) with borate. In support of this hypothesis, II has now been isolated. The reduction of scyllo-myo-inosose with NaBH<sub>4</sub> was reported (Reymond, C.A. 51, 12024c) to yield 32% I and 45% myoinositol (III). During this reduction the present author noted a white solid that began to precipitate from the mixture, and

after 24-36 hrs. this precipitate was collected, washed with H<sub>2</sub>O and dried to give

0.9 g. crude II. II was distinguished from I, III, and the starting material by paper chromatography. II migrated twice as fast as III on paper ionophoresis in 0.125M Na borate. I in this ionophoresis shows no migration. II is nonreducing in Fehling or Park-Johnson tests. II with Ac<sub>2</sub>O and H<sub>2</sub>SO<sub>4</sub> gave 60-70% I hexaacetate, m. 286°. III hexaacetate was not detected. II acidified with H<sub>2</sub>SO<sub>4</sub>, the resultant solution repeatedly evaporated with MeOH, the residue taken up in H<sub>2</sub>O, deionized

with Amberlite MB-3, and the eluate again taken to dryness gave I. II would appear to be a monohydrate. I heated at 100° with 0.125M borate gave a compound migrating at the same rate as II. The stereochemistry of II is still unproved and is being further investigated.

IT Scyllitol, diborate

RL: PREP (Preparation)

IT 488-59-5P, Scyllitol, Na derivative 892110-01-9P, Boric acid, ester with scyllitol

RL: PREP (Preparation)  
(preparation of)

L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:25260 CAPLUS

DOCUMENT NUMBER: 52:25260

ORIGINAL REFERENCE NO.: 52:4513i,4514a-i,4515a-g

TITLE: Cyclitols. VI. Hydrogenation of hexahydroxybenzene

AUTHOR(S): Anygal, S. J.; McHugh, D. J.

CORPORATE SOURCE: N.S. Wales Univ. Technol., Sydney

SOURCE: Journal of the Chemical Society (1957) 3682-91

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 51, 12010g. Catalytic hydrogenation of hexahydroxybenzene (I) under various conditions gave complex mixts. of polyhydroxycyclohexanes which were separated by chromatog. on cellulose powder. Seven inositols and 4 quercitols were obtained from various runs, including the previously unknown cis-inositol (II), cis-quercitol (III), and cis-inosose (IV). At room temperature with a Pd catalyst myo-inositol (V) was the chief product, whereas Pd-C gave mainly II. High temperature hydrogenation over

Raney

Ni showed little stereospecificity. Me2CO-H2O (4:1) was used as the mobile phase unless otherwise stated. A suspension of 4 g. tetrahydroxybenzoquinone (Va) and 0.2 g. 10% Pd-C in 250 mL. H2O hydrogenated at room temperature and pressure gave in 7 h. I, whereupon 1.0 g. Pd catalyst was added and the hydrogenation continued. The reduction required 82 h. and 3 g. more catalyst was added during this period, the catalyst was removed, washed with hot H2O and the filtrate evaporated under reduced pressure and dried. The partially crystallized residue was warmed with H2O, and the material filtered to give scyllo-inositol (VI), m. 330-40° (H2O-alc.); hexaacetyl derivative, m. 292-3°. The filtrate from VI was seeded with neo-inositol (VII) and left overnight at 0°, and the solution chromatographed on cellulose powder to give a mixture of inositols and V. Their isolation was further studied. Thus, fractions 20-36 contained a reducing compound which, when treated with PhNHNH2, gave IV phenylhydrazone, decomposing at 150-60° (MeOH-H2O). The phenylhydrazones gave IV, m. 179-80° (H2O-alc.) (decomposition). The mother liquors from the separation of the phenylhydrazones were freed from PhNHNH2 by warming with BzH and extracting with Et2O, evaporated, and the

residue

chromatographed, and after many chromatog. sepns. gave 7 fractions (A-G). Each fraction was evaporated to a small volume, treated with C, dissolved in a min. of alc. or aqueous alc., and stored at 0°. If no crystallization occurred, the solution was evaporated, the residue acetylated and stored under

a

min. of alc. Fraction A, RF 0.85, after acetylation gave crystals of cyclohexanetetrol tetraacetate (VIIa), m. 124° (EtOAc-ligroine). Deacetylation of VIIa by refluxing with alc. containing 5% HCl gave crystals, darkening at 195-200°, m. 205-10°. The residue from the mother liquors gave a mixture of noncryst. cyclohexanetetrol tetraacetates.

Fraction B, RF 0.70, could not be crystallized. In another run (from Va) this fraction showed strong reducing properties and after further chromatog. gave a pure product, m. 160-1°, which reduced Fehling solution in the cold, and failed to give a crystalline acetate. The RF of fractions C, D, and E was 0.62, 0.53, and 0.45, resp. No crystalline product could be obtained. After acetylation, each fraction was distilled in vacuo. Anal. showed the first 2 to be mixts. of tetraacetoxycyclohexanes and the last a mixture of penta-O-acetylquercitols. From fraction F (RF 0.39) crystals separated; acetylation gave penta-O-acetyl-cis-quercitol (VIII), m. 162.5° (alc.-H<sub>2</sub>O). Hydrolysis of VIII followed by sublimation gave III, m. 235-40° (decomposition). The mother liquors of the III fraction after several weeks gave epiquercitol (IX), m. 206-9° (decomposition); acetylation gave penta-O-acetylepiquercitol, m. 141-2°. From fraction G (RF 0.31) a few crystals separated; acetylation followed by sublimation gave scyllo-quercitol acetate, m. 193-4°, and hydrolysis gave scyllo-quercitol (X), m. 235°. The mother liquors of X gave no Scherer test, indicating the absence of allo-inositol (XI). Fractions 44-75 of the preliminary separation were found by paper chromatog. to contain II, epi- (XII), and (±)-inositol (XIII). Since II and XII had the same RF value in Me<sub>2</sub>CO-H<sub>2</sub>O, the mixture was dissolved in BuOH-AcOH-H<sub>2</sub>O (4:1:1), after 2 days XIII separating; acetylation gave a product, m. 110°. The mother liquors from XIII chromatographed in the same solvent ratio gave after crystallization II; the hexaacetate, m. 208° (alc. H<sub>2</sub>O), hydrolyzed gave II. II decomposed on slow heating but m. 377° (decomposition); hexabenzate, m. 252° (anhydrous alc.). The fractions containing mainly XII were combined and acetylated to give epi-inositol acetate which after sublimation m. 187°. Fractions 76-250 gave V, m. 222-4° (aqueous alc.). IV (18 mg.) hydrogenated 3 h. in N HCl over 5 mg. PtO<sub>2</sub> and the product chromatographed, and then acetylated gave II acetate. The quercitol fraction acetylated gave VIII, identical with the sample obtained from the hydrogenation of Va. A small scale hydrogenation in H<sub>2</sub>O with PtO<sub>2</sub> followed by paper chromatog. showed the formation of II accompanied by traces of XII. IV (50 mg.) in 3 mL H<sub>2</sub>O, kept slightly acid by addition of N H<sub>2</sub>SO<sub>4</sub>, treated with 1 g. Na-Hg gave XII penta-O-acetate. Va (10 g.), 6 g. Raney Ni W-2, 100 mL alc., and 70 mL H<sub>2</sub>O hydrogenated 40 min. at 120°/150 atmospheric and then 0.5 h. at 140°, the solution filtered, concentrated in vacuo, and dried gave a residue which, diluted with MeOH, m. about 280°, and V, m. 218-20°. Acetylation of the material gave VII hexaacetate, m. 254°; sublimation of the alc.-insol. residue gave VI hexaacetate. The filtrate from VI and VII was chromatographed and the products grouped in fractions A-F. Fraction A (RF 0.77) gave all-cis-cyclohexane-1,2,3-triol, m. 146-7°; hexabenzate, m. 145°. Fractions B (RF 0.61) and D (RF 0.44) gave no crystalline products. Fraction C (RF 0.55) after crystallization and sublimation gave fractions m. 135-45°, 177-87°, 197-225°, and 225-7°. No pure substances were obtained. Fraction E (RF 0.39) gave III; acetate, m. 163°. There was no evidence of muco-inositol being present. Fraction F (RF 0.33) gave IX; acetate, m. 140°, also a form m. 122-3°. The mother liquors from IX were evaporated and chromatographed to give X acetate, and deacetylation yielded X, m. 232°. The mother liquors were concentrated to give allo-inositol acetate, m. 142°. Fractions 51-70 of the preliminary separation which contained II and XII on crystallization gave XII and II.

Fractions 38-50 were rechromatographed and crystallized to give II. All the mother liquors of fractions 38-70 were rechromatographed to give a mixture of IX and X, crude II, and crude XII. There was no evidence for the presence of XIII. Fractions 76-100 of the preliminary separation gave V. A

suspension of Va and 1 g. Pd-C in 200 mL. H<sub>2</sub>O hydrogenated 110 h., and paper chromatographed showed a high concentration of V and III and weaker spots at RF 0.31 and 0.38. Evaporation gave a resin which on crystallization gave

VI. The solution was decanted, evaporated, dissolved in H<sub>2</sub>O, diluted with Me<sub>2</sub>CO, and chromatographed. Fractions 21-50 were rechromatographed to give III. Nearly all the II was in fractions 51-150; recrystn. gave pure II. The mother liquors were rechromatographed to give 3 main fractions. The first contained chiefly II, its mother liquors gave XIII. The 2nd fraction gave pure II and a mixture of II and XII. The 3rd fraction was chiefly V. All the mother liquors were again chromatographed and the first product acetylated gave X acetate. The 2nd half containing II and XII on acetylation gave XII acetate, m. 187-8°. The contents of fractions 181-260 fractionally crystallized gave VI and the remainder combined with fractions 151-180 gave IV. Va (10 g.) in 150 mL. H<sub>2</sub>O was hydrogenated 2 h. with Pd-C, the hexahydrobenzene precipitated, and reduced at 100 atmospheric over 10 g. more

catalyst and 100 mL. H<sub>2</sub>O; after 23 h. the reduction was still incomplete so that the mixture was further hydrogenated 19 h. at 45-50°, and the isolated product gave 8.4 g. crude material, which left VI when redissolved in a little H<sub>2</sub>O. The filtrate was diluted with 300 mL. H<sub>2</sub>O and shaken 20 min. with 200 g. of strong base anion exchange resin converted into the borate form; paper chromatog. showed that all II had been removed but some IV and VI and unidentified material remained. The solution was filtered and the filtrate was not worked up. After the resin was shaken 1 h. with H<sub>2</sub>O, the filtrate contained IV. Repetition of this process 20 times still gave IV in the filtrate. The combined washings on evaporation and crystallization gave chiefly IV and another compound

Chromatog. and acetylation gave a quercitol pentaacetate, m. 115-17°, which after deacetylation gave a quercitol, decomposing at 230-40°, which was not identical with any known quercitol. The resin shaken twice with 400 mL. N HCl gave first VI, then II, the mother liquors containing III and IX (or X), II, XII, and IV. III and II were isolated by chromatog. The other fractions were not worked up.

AB cf. C.A. 51, 12010g. Catalytic hydrogenation of hexahydroxybenzene (I) under various conditions gave complex mixts. of polyhydroxycyclohexanes which were separated by chromatog. on cellulose powder. Seven inositols and 4 quercitols were obtained from various runs, including the previously unknown cis-inositol (II), cis-quercitol (III), and cis-inosose (IV). At room temperature with a Pd catalyst myo-inositol (V) was the chief product, whereas Pd-C gave mainly II. High temperature hydrogenation over

Raney Ni showed little stereospecificity. Me<sub>2</sub>CO-H<sub>2</sub>O (4:1) was used as the mobile phase unless otherwise stated. A suspension of 4 g. tetrahydroxybenzoquinone (Va) and 0.2 g. 10% Pd-C in 250 mL. H<sub>2</sub>O hydrogenated at room temperature and pressure gave in 7 h. I, whereupon 1.0 g. Pd catalyst was added and the hydrogenation continued. The reduction required 82 h. and 3 g. more catalyst was added during this period, the catalyst was removed, washed with hot H<sub>2</sub>O and the filtrate evaporated under reduced pressure and dried. The partially crystallized residue was warmed with H<sub>2</sub>O, and the material filtered to give scyllo-inositol (VI), m. 330-40° (H<sub>2</sub>O-alc.); hexaacetyl derivative, m. 292-3°. The filtrate from VI was seeded with neo-inositol (VII) and left overnight at 0°, and the solution chromatographed on cellulose powder to give a mixture of inositols and V. Their isolation was further studied. Thus, fractions 20-36 contained a reducing compound which, when treated with PhNNH<sub>2</sub>, gave IV phenylhydrazone, decomposing at 150-60° (MeOH-H<sub>2</sub>O). The phenylhydrazone gave IV, m. 179-80° (H<sub>2</sub>O-alc.) (decomposition). The

mother liquors from the separation of the phenylhydrazone were freed from PhNHNH<sub>2</sub> by warming with BzH and extracting with Et<sub>2</sub>O, evaporated, and the residue

chromatographed, and after many chromatog. sepsns. gave 7 fractions (A-G). Each fraction was evaporated to a small volume, treated with C, dissolved in a min. of alc. or aqueous alc., and stored at 0°. If no crystallization occurred, the solution was evaporated, the residue acetylated and stored under

a min. of alc. Fraction A, RF 0.85, after acetylation gave crystals of cyclohexanetetrol tetraacetate (VIIa), m. 124° (EtOAc-ligroine). Deacetylation of VIIa by refluxing with alc. containing 5% HCl gave crystals, darkening at 195-200°, m. 205-10°. The residue from the mother liquors gave a mixture of noncryst. cyclohexanetetrol tetraacetates. Fraction B, RF 0.70, could not be crystallized. In another run (from Va) this fraction showed strong reducing properties and after further chromatog. gave a pure product, m. 160-1°, which reduced Fehling solution in the cold, and failed to give a crystalline acetate. The RF of fractions C, D, and E was 0.62, 0.53, and 0.45, resp. No crystalline product could be obtained. After acetylation, each fraction was distilled in vacuo. Anal. showed the first 2 to be mixts. of tetraacetoxycyclohexanes and the last a mixture of penta-O-acetylquercitols. From fraction F (RF 0.39) crystals separated; acetylation gave penta-O-acetyl-cis-quercitol (VIII), m. 162.5° (alc.-H<sub>2</sub>O). Hydrolysis of VIII followed by sublimation gave III, m. 235-40° (decomposition). The mother liquors of the III fraction after several weeks gave epiquercitol (IX), m. 206-9° (decomposition); acetylation gave penta-O-acetylepiquercitol, m. 141-2°. From fraction G (RF 0.31) a few crystals separated; acetylation followed by sublimation gave scyllo-quercitol acetate, m. 193-4°, and hydrolysis gave scyllo-quercitol (X), m. 235°. The mother liquors of X gave no Scherer test, indicating the absence of allo-inositol (XI). Fractions 44-75 of the preliminary separation were found by paper chromatog. to contain II, epi- (XII), and (±)-inositol (XIII). Since II and XII had the same RF value in Me<sub>2</sub>CO-H<sub>2</sub>O, the mixture was dissolved in BuOH-AcOH-H<sub>2</sub>O (4:1:1), after 2 days XIII separating; acetylation gave a product, m. 110°. The mother liquors from XIII chromatographed in the same solvent ratio gave after crystallization II; the hexaacetate, m. 208° (alc. H<sub>2</sub>O), hydrolyzed gave II. II decomposed on slow heating but m. 377° (decomposition); hexabenzozoate, m. 252° (anhydrous alc.). The fractions containing mainly XII were combined and acetylated to give epi-inositol acetate which after sublimation m. 187°. Fractions 76-250 gave V, m. 222-4° (aqueous alc.). IV (18 mg.) hydrogenated 3 h. in N HCl over 5 mg. PtO<sub>2</sub> and the product chromatographed, and then acetylated gave II acetate. The quercitol fraction acetylated gave VIII, identical with the sample obtained from the hydrogenation of Va. A small scale hydrogenation in H<sub>2</sub>O with PtO<sub>2</sub> followed by paper chromatog. showed the formation of II accompanied by traces of XII. IV (50 mg.) in 3 mL H<sub>2</sub>O, kept slightly acid by addition of N H<sub>2</sub>SO<sub>4</sub>, treated with 1 g. Na-Hg gave XII penta-O-acetate. Va (10 g.), 6 g. Raney Ni W-2, 100 mL. alc., and 70 mL. H<sub>2</sub>O hydrogenated 40 min. at 120°/150 atmospheric and then 0.5 h. at 140°, the solution filtered, concentrated in vacuo, and dried gave a residue which, diluted with MeOH, m. about 280°, and V, m. 218-20°. Acetylation of the material gave VII hexaacetate, m. 254°; sublimation of the alc.-insol. residue gave VI hexaacetate. The filtrate from VI and VII was chromatographed and the products grouped in fractions A-F. Fraction A (RF 0.77) gave all-cis-cyclohexane-1,2,3-triol, m. 146-7°; hexabenzozoate, m. 145°. Fractions B (RF 0.61) and D (RF 0.44) gave no crystalline products. Fraction C (RF 0.55) after crystallization and sublimation gave fractions m. 135-45°, 177-87°,



197-225°, and 225-7°. No pure substances were obtained. Fraction E (RF 0.39) gave III; acetate, m. 163°. There was no evidence of muco-inositol being present. Fraction F (RF 0.33) gave IX; acetate, m. 140°, also a form m. 122-3°. The mother liquors from IX were evaporated and chromatographed to give X acetate, and deacetylation yielded X, m. 232°. The mother liquors were concentrated to give allo-inositol acetate, m. 142°. Fractions 51-70 of the preliminary separation which contained II and XII on crystallization gave XII

and II.

Fractions 38-50 were rechromatographed and crystallized to give II. All the mother liquors of fractions 38-70 were rechromatographed to give a mixture of IX and X, crude II, and crude XII. There was no evidence for the presence of XIII. Fractions 76-100 of the preliminary separation gave V. A suspension of Va and 1 g. Pd-C in 200 mL H<sub>2</sub>O hydrogenated 110 h., and paper chromatographed showed a high concentration of V and III and weaker spots at RF 0.31 and 0.38. Evaporation gave a resin which on crystallization gave

VI. The

solution was decanted, evaporated, dissolved in H<sub>2</sub>O, diluted with Me<sub>2</sub>CO, and chromatographed. Fractions 21-50 were rechromatographed to give III. Nearly all the II was in fractions 51-150; recrystn. gave pure II. The mother liquors were rechromatographed to give 3 main fractions. The first contained chiefly II, its mother liquors gave XIII. The 2nd fraction gave pure II and a mixture of II and XII. The 3rd fraction was chiefly V. All the mother liquors were again chromatographed and the first product acetylated gave X acetate. The 2nd half containing II and XII on acetylation gave XII acetate, m. 187-8°. The contents of fractions 181-260 fractionally crystallized gave VI and the remainder combined with fractions 151-180 gave IV. Va (10 g.) in 150 mL H<sub>2</sub>O was hydrogenated 2 h. with Pd-C, the hexahydrobenzene precipitated, and reduced at 100 atmospheric over

10 g. more

catalyst and 100 mL H<sub>2</sub>O; after 23 h. the reduction was still incomplete so that the mixture was further hydrogenated 19 h. at 45-50°, and the isolated product gave 8.4 g. crude material, which left VI when redissolved in a little H<sub>2</sub>O. The filtrate was diluted with 300 mL H<sub>2</sub>O and shaken 20 min. with 200 g. of strong base anion exchange resin converted into the borate form; paper chromatog. showed that all II had been removed but some IV and VI and unidentified material remained. The solution was filtered and the filtrate was not worked up. After the resin was shaken 1 h. with H<sub>2</sub>O, the filtrate contained IV. Repetition of this process 20 times still gave IV in the filtrate. The combined washings on evaporation and crystallization gave chiefly IV and another compound

Chromatog. and

acetylation gave a quercitol pentaacetate, m. 115-17°, which after deacetylation gave a quercitol, decomposing at 230-40°, which was not identical with any known quercitol. The resin shaken twice with 400 mL N HCl gave first VI, then II, the mother liquors containing III and IX (or X), II, XII, and IV. III and II were isolated by chromatog. The other fractions were not worked up.

IT 1,2,3-Cyclohexanetriol, cis-

RL: PREP (Preparation)

IT 488-59-5P, Scyllitol 20021-56-1P, 1,2,3,4-Cyclohexanetetrol, tetraacetate 20108-52-5P, Scyllitol, hexaacetate 92298-56-1P, 1,2,3,5-Cyclohexanetetrol, tetraacetate 92298-57-2P, 1,2,4,5-Cyclohexanetetrol, tetraacetate 96069-08-8P, 1,2,3-Cyclohexanetriol, tribenzoate

RL: PREP (Preparation)

(preparation of)

IT 13124-19-1P, Inosose

RL: PREP (Preparation)

(stereoisomers, formation in hydrogenation of benzenehexol, and derivs.)

IT 87-89-8P, Inositol 62076-18-0P, Quercitol  
 RL: PREP (Preparation)  
 (stereoisomers, formation in hydrogenation of benzenehexol, and esters)

L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1957:66483 CAPLUS  
 DOCUMENT NUMBER: 51:66483  
 ORIGINAL REFERENCE NO.: 51:12024c-d  
 TITLE: Cyclitol series. XXIII. The reduction of two inososes by sodium borohydride  
 AUTHOR(S): Reymond, D.  
 CORPORATE SOURCE: Univ. Geneva, Switz.  
 SOURCE: Helvetica Chimica Acta (1957), 40, 492-4  
 CODEN: HCACAV; ISSN: 0018-019X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: French

AB cf. C.A. 50, 1618h. Scyllo-ms-inosose and NaBH<sub>4</sub> 18 hrs. at room temperature give 45% ms-inositol and 32% scyllitol. Similarly, DL-epi-ms-inosose gives 90% epiinositol and no ms-inositol. A mechanism is suggested.

TI Cyclitol series. XXIII. The reduction of two inososes by sodium borohydride

AB cf. C.A. 50, 1618h. Scyllo-ms-inosose and NaBH<sub>4</sub> 18 hrs. at room temperature give 45% ms-inositol and 32% scyllitol. Similarly, DL-epi-ms-inosose gives 90% epiinositol and no ms-inositol. A mechanism is suggested.

IT Inosose, scyllo-meso-  
 (reduction with NaBH<sub>4</sub>)

IT 16940-66-2, Sodium borohydride  
 (inosose reduction by)

IT 488-59-5P, Scyllitol  
 RL: PREP (Preparation)  
 (preparation of)

IT 13124-19-1, Inosose, DL-epi-meso-  
 (reduction with NaBH<sub>4</sub>)

IT 87-89-8P, Inositol  
 RL: PREP (Preparation)  
 (stereoisomers, preparation of)

=> logoff hold  
 COST IN U.S. DOLLARS  
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
39.35	49.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  
 CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
-7.20	-7.20

SESSION WILL BE HELD FOR 120 MINUTES  
 STN INTERNATIONAL SESSION SUSPENDED AT 10:27:17 ON 28 MAY 2008